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Explicit Runge–Kutta methods for initial value problems with oscillating solutions

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Abstract

New pairs of embedded Runge–Kutta methods specially adapted to the numerical solution of first order systems of differential equations which are assumed to possess oscillating solutions are obtained. These pairs have been derived taking into account not only the usual properties of accuracy, stability and reliability of the local error estimator to adjust the stepsize of the underlying formulas but also the dispersion and dissipation orders of the advancing formula as defined by Van der Houwen and Sommeijer (1989). Three nine-stage embedded pairs of Runge–Kutta methods with algebraic orders 7 and 5 and higher orders of dispersion and/or dissipation are selected among the members of a family of pairs depending on several free parameters. Some numerical results are presented to show the efficiency of the new methods.

Keywords: Runge–Kutta methods; Periodic initial value problems; Dispersion and dissipation errors

AMS classification: 65L05

1. Introduction

In recent years, several papers proposing Runge–Kutta (RK) type methods for the numerical solution of ODEs with oscillating solutions have been published. Among them we may mention the pioneer paper of Brusa and Nigro [1], in which for the first time the phase-lag property was introduced as a tool to analyze the behaviour of a method for the numerical solution of ODEs with oscillating solutions. Moreover, these authors derived a third order implicit RK method with suitable phase-lag properties to be used in structural dynamics.

Next, Van der Houwen and Sommeijer in a number of papers [10–12] introduced a precise theoretical framework to analyze the behaviour of numerical methods for oscillatory problems. Thus, for RK methods, by using the linear test problem $y' = i\omega y$, $\omega \in \mathbb{R}$ and a fixed stepsize h they defined the dispersion (or phase-lag) error as the error in the phase of the numerical solution and

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the dissipation (or amplification) error as the error in the numerical damping. Since these errors can be written in terms of the product $\omega h = v$, if the dispersion (resp. dissipation) error is $O(v^{q+1})$, $(v \to 0)$ the method is said to be dispersive (resp. dissipative) of order q. A similar study was also carried out for RK Nyström methods with respect to the usual test equation for second order oscillatory problems: $y'' + \omega^2 y = 0$. As these authors pointed out, methods with higher orders of dispersion are suitable for long time integration of oscillating solutions because the stepsizes can be chosen larger than in conventional methods and moreover the global errors show a more favourable propagation along the integration interval.

Runge–Kutta schemes with low-dispersion and dissipation have been also considered by Hu et al. (see [6] and the references cited therein) in connection with the numerical solution of differential equations arising in computational accoustics. As remarked by these authors, in many CFD applications RK schemes have the advantage of their low storage requirements and relative large stability limits. However, for computing acoustic waves the stability alone is not sufficient and nondissipative and nondispersive properties are of critical importance. Due to this fact several RK methods with four, five and six stages and low-dispersion and dissipation properties have been proposed in [6] for computation of acoustic waves.

A remarkable fact is that almost all RK formulas with higher dispersive and/or dissipative orders proposed in the last years have been designed to be used with a fixed stepsize. To our knowledge, only two exceptions have appeared in the literature. First, a recent paper of Sideris and Simos [9] which considers variable stepsize RK methods, with phase-lag orders four or six, based on a modification of the classical RK Fehlberg pair 3(4). Secondly, a paper of Sharp et al. [8] in which several pairs of diagonally implicit RK Nyström methods are obtained with the aim to be used in the numerical solution of second order ODEs with oscillating solutions with a wide range of frequencies. However, since it is well known that all practical codes for the numerical solution of ODEs have the possibility to vary the stepsize at each step to get a more accurate and efficient integration, it seems clear that practical methods for oscillating solutions should also include such a reliable local error estimate to adjust the stepsize according to a given tolerance. Such error estimate is obtained usually from a pair of RK formulas as shown in [2, 5].

On the other hand, let us remark that most explicit RK pairs of higher orders presented in the last years have been obtained taking as starting point a family of pairs depending on several parameters and then selecting an optimal pair attending the properties of accuracy, stability and a reliable error estimate. The approach of this paper follows this way in the construction of a family of pairs but differs from the standard approach in the sense that, to select optimal pairs, we have taken into account not only the above properties but also the dispersion and/or dissipation properties which, as remarked above, play an important role in the numerical integration of problems with oscillating solutions. In this way new methods have been obtained that share the good accuracy and stability behaviour typical of most high order RK methods, together with the advantages derived from the accuracy of the phase-lag and dissipation properties for oscillating solutions.

The paper is organised as follows: In Section 2 we summarize some properties on the dispersion, dissipation and algebraic orders of RK methods which are relevant to our study. In particular, simple sets of conditions on the coefficients of the RK formula for given orders of dispersion and dissipation are presented. In Section 3 we describe briefly the construction of a family of embedded pairs with nine stages depending on five free parameters and we discuss how to choose these parameters in order to achieve the highest phase-lag and/or dissipation orders. As a consequence

of this study dissipative and/or dispersive optimal order methods are derived. Finally, in Section 4, some conclusions on the numerical performance of these methods are presented. In particular, by testing the behaviour of the new selected pairs with a wide variety of oscillating problems we have found as numerically optimal a pair which is dispersive of order 10 and dissipative of order 9. In addition, numerical comparisons between codes based in the new optimal pair and the higher order pairs of Fehlberg [4], and Prince and Dormand [7] are also presented.

2. Dispersive, dissipative and algebraic order conditions of RK methods

We consider a first order initial value problem

$$y' = f(t, y), \quad y(t_0) = y_0, \quad t \in [t_0, t_{\text{end}}], \tag{2.1}$$

which is assumed to possess an oscillatory solution $y = y(t)$ and where $f(t, y)$ is sufficiently smooth in a neighbourhood of this solution $(t, y(t)); t \in [t_0, t_{\text{end}}]$.

Let $A = (a_{ij}) \in \mathbb{R}^{s \times s}$, $\boldsymbol{b} = (b_i) \in \mathbb{R}^s$ and $\boldsymbol{b}^* = (b_i^*) \in \mathbb{R}^s$ be the coefficients of a RK pair of formulas with s stages written in terms of the usual Butcher's notation. For a given approximation y_n to the solution of (2.1) at t_n, $y(t_n)$, this pair of formulas produces two new approximations y_{n+1} and y_{n+1}^* to $y(t_{n+1})$, $(t_{n+1} = t_n + h_n)$, of orders p and $p^* < p$, according to

$$y_{n+1} = y_n + h_n \sum_{j=1}^{s} b_j f(t_n + c_j h_n, Y_{n,j}), \tag{2.2}$$

$$y_{n+1}^* = y_n + h_n \sum_{j=1}^{s} b_j^* f(t_n + c_j h_n, Y_{n,j}), \tag{2.3}$$

where $c_i = \sum_{j=1}^{s} a_{ij}$, $i = 1, \ldots, s$ and

$$Y_{n,j} = y_n + h_n \sum_{i=1}^{s} a_{ji} f(t_n + c_i h_n, Y_{n,i}), \quad j = 1, \ldots, s. \tag{2.4}$$

In the remainder of this paper we restrict our considerations to explicit methods. Then A is a lower triangular matrix and the stages $Y_{n,j}$ can be computed explicitly from (2.4).

Denoting by $y_n(t) = y(t; t_n, y_n)$ the local solution of $y' = f(t, y)$ at the point (t_n, y_n), the formula (2.2), (2.4) has algebraic order p if $|y_{n+1} - y_n(t_{n+1})| = O(h_n^{p+1})$ holds for all f sufficiently smooth. The conditions to be satisfied by the coefficients $(A, \boldsymbol{b})$ of the formula (2.2), (2.4) for a given order p can be found e.g. in [2] and have the form

$$\boldsymbol{b}^{\mathrm{T}} \Phi_j = 1/\gamma_j, \quad j = 1, \ldots, N_p,$$

where $\Phi_j = \Phi_j(A) \in \mathbb{R}^s$ are polynomic functions on the coefficients a_{ij} of the method, γ_j are fixed positive integers and N_p the number of independent equations to be satisfied for a given method to have order p.

In our study we are interested in an embedded pair of formulas (2.2)–(2.4) with nine-stages and orders 7 and 5, respectively. Since both formulas share the same matrix A, the algebraic order

conditions on the coefficients of the pair will be

$$\boldsymbol{b}^{\mathrm{T}}\Phi_j = 1/\gamma_j, \quad j = 1,\ldots,N_7, \ N_7 = 85, \tag{2.5}$$

for the solution of order seven and

$$\boldsymbol{b}^{*\mathrm{T}}\Phi_j = 1/\gamma_j, \quad j = 1,\ldots,N_5, \ N_5 = 17, \tag{2.6}$$

for the solution of order five with $\boldsymbol{b}, \boldsymbol{b}^*$ and $\Phi_j \in \mathbb{R}^9$.

The RK pair will be applied in local extrapolation mode. This means that the integration advances with the higher order formula (2.2), (2.4), while the lower order approximation y^*_{n+1} given by (2.3) is used only to control the local error in the current step and to monitor the variable stepsize in the usual way (see e.g. [5, 7]). In view of these remarks the analysis of the phase and dissipation properties of the method will be referred to the higher order formula (2.2), (2.4).

Following [10] we introduce next the so called dispersion and dissipation errors of the RK formula $(A, \boldsymbol{b})$ defined by (2.2), (2.4) by testing it with linear homogeneous scalar equations $y' = \mathrm{i}\omega y$, where $\mathrm{i} = \sqrt{-1}$, ω is a real constant and assuming that the formula advances with a fixed stepsize $h = h_n$. It is worth to remark that Van der Houwen and Sommeijer have shown in [11] that for the inhomogeneous test equation $y' = \mathrm{i}\omega y + c\exp(\mathrm{i}\omega_{\mathrm{p}} t)$, $(\omega_{\mathrm{p}} \neq \omega)$ with a nonresonant periodic forcing term and over long integration intervals, the error introduced by the homogeneous component of the numerical solution is the more important source of error whereas the error in the inhomogeneous component does not increases. As a consequence of this fact, our study will be restricted to linear homogeneous test equations.

For the homogeneous test equation the numerical solution provided by (2.2), (2.4) is

$$y_{n+1} = R(\mathrm{i}v) y_n,$$

where $v = h\omega$ and

$$R(\mathrm{i}v) = 1 + \mathrm{i}v\boldsymbol{b}^{\mathrm{T}}(I - \mathrm{i}vA)^{-1}\boldsymbol{e}, \tag{2.7}$$

with $\boldsymbol{e} = (1,\ldots,1)^{\mathrm{T}} \in \mathbb{R}^s$. On the other hand for the exact solution we have $y(t_{n+1}) = \mathrm{e}^{\mathrm{i}v} y(t_n)$. A comparison of the factors $R(\mathrm{i}v)$ and $\mathrm{e}^{\mathrm{i}v}$ associated to the numerical and the exact solutions leads to the following:

Definition 2.1. The RK formula (2.2), (2.4) (and also the pair of formulas) is said to be

- Dispersive of order q if $\phi(v) := v - \arg(R(\mathrm{i}v)) = \mathrm{O}(v^{q+1}), \quad (v \to 0).$ (2.8)
- Dissipative of order r if $\alpha(v) := 1 - |R(\mathrm{i}v)| = \mathrm{O}(v^{r+1}), \quad (v \to 0).$ (2.9)

In addition, the functions $\phi(v)$ and $\alpha(v)$ are called the dispersion and dissipation error functions.

It must be noticed that for an explicit method with s stages $A^s \equiv 0$, and therefore $R(\mathrm{i}v)$ is a polynomial in v of degree $\leqslant s$ which can be written in the form

$$R(\mathrm{i}v) = \sum_{j=0}^{s} \beta_j (\mathrm{i}v)^j, \tag{2.10}$$

where β_j are real scalars given by

$$\beta_0 = 1, \qquad \beta_j = \boldsymbol{b}^{\mathrm{T}} A^{j-1} \boldsymbol{e} \quad (j \geqslant 1). \tag{2.11}$$

To derive the conditions to be satisfied by the β_j for a given order of dissipation note that $\alpha(v)[1 + |R(\mathrm{i}v)|] = 1 - |R(\mathrm{i}v)|^2$ is an even function of v and therefore its power series expansion around the origin has the form

$$\alpha(v)[1 + |R(\mathrm{i}v)|] = D_0 + D_2 v^2 + D_4 v^4 + \cdots \tag{2.12}$$

with $D_0 = 0$. Moreover, it follows from (2.10) that

$$|R(\mathrm{i}v)|^2 = R(\mathrm{i}v)R(-\mathrm{i}v) = \sum_{l=0}^{s} (-1)^l \left(\sum_{k=0}^{2l} \beta_{2l-k}\beta_k (-1)^k \right) v^{2l},$$

where $\beta_j = 0$, $j > s$. Then, the coefficients D_j are given by $D_0 = 0$, and

$$D_{2l} = (-1)^{l+1} \sum_{k=0}^{2l} \beta_{2l-k}\beta_k (-1)^k. \tag{2.13}$$

As a consequence of (2.9), (2.12) we can state the following:

Property 2.2. *The explicit RK formula* (2.2), (2.4) *is dissipative of order* $r = 2r' + 1$ *if and only if the coefficients* D_{2j} *given by* (2.13) *satisfy*

$$D_2 = \cdots = D_{2r'} = 0, \qquad D_{2r'+2} \neq 0.$$

Moreover, $\frac{1}{2}(D_{2r'+2})$ *is the coefficient of the leading term of the error dissipation* $\alpha(v)$ *in* (2.9).

Concerning the order of dispersion a study of the power series expansion of the function $\phi(v)$ in terms of the coefficients β_j leads to the following:

Property 2.3. *The explicit RK formula defined by* (2.2), (2.4) *is dispersive of order* $q = 2m$ *if the linear homogeneous functionals* $C_{2j+1} = C_{2j+1}(\beta_0, \ldots, \beta_{2j+1})$, $(j \geqslant 0)$ *defined by*

$$C_{2j+1} = C_{2j+1}(\beta_0, \ldots, \beta_{2j+1}) = iv(-1)^j \sum_{i=0}^{2j+1} \frac{(-1)^i \beta_i}{(2j+1-i)!}, \tag{2.14}$$

satisfy

$$C_1 = C_3 = \cdots = C_{2m-1} = 0, \quad C_{2m+1} \neq 0. \tag{2.15}$$

Moreover, if the constant $C_{2m+1} \neq 0$, *it is the coefficient of the leading term of the error of dispersion* $\phi(v)$ *in* (2.8).

Proof. Collecting separately the real and imaginary parts of $R(\mathrm{i}v)$ in (2.10) we have

$$R(\mathrm{i}v) = A(v^2) + \mathrm{i}vB(v^2),$$

where A and B are polynomials in v^2 of degrees $s' = [s/2]$ and $s'' = [(s+1)/2] - 1$, respectively, and their coefficients are given in terms of β_j by

$$A(v^2) = \sum_{j=0}^{s'} (-1)^j \beta_{2j} v^{2j}, \quad vB(v^2) = \sum_{j=0}^{s''} (-1)^j \beta_{2j+1} v^{2j+1}. \tag{2.16}$$

Then, the dispersion error function (2.8) can be written as

$$\phi(v) = v - \arctan\left(\frac{vB(v^2)}{A(v^2)}\right), \quad (A(v^2) \neq 0)$$

which is clearly an odd function of v. Thus, the method is dispersive of order $2m$ if

$$v - \arctan\left(\frac{vB(v^2)}{A(v^2)}\right) \simeq Cv^{2m+1}, \quad (v \to 0, C \neq 0)$$

which in view of $\beta_0 = 1$ is equivalent to

$$A(v^2)\sin v - vB(v^2)\cos v \simeq Cv^{2m+1}. \tag{2.17}$$

Substituting the power series of $A, B, \sin v, \cos v$ into the left-hand side of (2.17) we get

$$A(v^2)\sin v - vB(v^2)\cos v = \sum_{l \geqslant 0} C_{2l+1} v^{2l+1},$$

with the coefficients C_{2j+1} given by (2.14). Then the method is dispersive of order $2m$ if (2.15) holds and $C = C_{2m+1}$.

Note that conditions (2.15) on the β_j exhibit a remarkable simplicity: each coefficient C_{2j+1} is, apart of its sign $(=(-1)^j)$, a sum of all possible terms of type $(-1)^l \beta_l / m!$ with $l + m = 2j + 1$. In particular, for the first orders of dispersion we have

Order 2: $C_1 = \beta_0 - \beta_1 = 0,$

Order 4: $-C_3 = \left(\frac{\beta_0}{3!} + \frac{\beta_2}{1!}\right) - \left(\frac{\beta_1}{2!} + \frac{\beta_3}{0!}\right) = 0,$

Order 6: $C_5 = \left(\frac{\beta_0}{5!} + \frac{\beta_2}{3!} + \frac{\beta_4}{1!}\right) - \left(\frac{\beta_1}{4!} + \frac{\beta_3}{2!} + \frac{\beta_5}{0!}\right) = 0.$

Further, it must be noticed that the conditions on the β_j given in the Property 2.3. are equivalent to those obtained by Van der Houwen and Sommeijer in [13, Theorem 2.1].

On the other hand, if $\beta_j = 1/j!$, $(j = 0, 1, \ldots, p)$ and $\beta_{p+1} \neq 1/(p+1)!$ with $p = 2p'$, then $C_1 = C_3 = \cdots = C_{2p'-1} = 0$ and $C_{2p'+1} \neq 0$, which implies that the order of dispersion is exactly $2p'$. However if $p = 2p' - 1$ is odd, we have $C_1 = C_3 = \cdots = C_{2p'-1} = 0$, since $C_{2p'+1}$ can be written as a function of $\beta_{2p'}$ and $\beta_{2p'+1}$, in this case the order of dispersion can be $\geqslant 2p'$ for suitable values of these parameters.

Next we restrict our attention to the class of methods that will be considered in the next section. They have nine stages and algebraic order seven, therefore $\beta_j = 1/j!$, $j \leqslant 7$ and $\beta_j = 0$ for $j \geqslant 10$, consequently

$$\begin{aligned} &D_2 = D_4 = D_6 = 0, \\ &D_8 = (-1)^5 \left[2\left(\beta_8 - \frac{1}{8!}\right)\right], \\ &D_{10} = (-1)^6 \left[-\frac{2}{10!} - 2\left(\beta_9 - \frac{1}{9!}\right) + 2\left(\beta_8 - \frac{1}{8!}\right)\frac{1}{2!}\right]. \end{aligned} \tag{2.18}$$

This implies that all methods will have order of dissipation $\geqslant 7$. Further if β_8 and β_9 have the values

$$\beta_8 = \frac{1}{8!}, \qquad \beta_9 = \frac{1}{10(8!)}, \tag{2.19}$$

then $D_8 = D_{10} = 0$ and $D_{12} \neq 0$ and the they have order of dissipation 11 which is actually the highest attainable order within this class of formulas.

For the dispersion properties of our methods we have $C_1 = C_3 = C_5 = C_7 = 0$ and they have at least order of dispersion 8. They will attain a higher order if there exists $k \geqslant 4$ such that $C_{2j+1} = 0$, for $k \geqslant j \geqslant 4$. The calculation of these coefficients can be done easily taking into account that if $\beta_l = 1/l!$ for $l = 0, \ldots, 7$. Clearly, $C_{2j+1}(\beta_0, \ldots, \beta_{2j+1}) = 0$, for $j = 0, \ldots, 3$ and therefore for these methods we have

$$\begin{aligned} &+C_9 = \left(\beta_8 - \frac{1}{8!}\right) - \left(\beta_9 - \frac{1}{9!}\right), \\ &-C_{11} = \frac{1}{3!}\left(\beta_8 - \frac{1}{8!}\right) - \frac{1}{2!}\left(\beta_9 - \frac{1}{9!}\right) - \frac{1}{10!} + \frac{1}{11!}, \\ &+C_{13} = \frac{1}{5!}\left(\beta_8 - \frac{1}{8!}\right) - \frac{1}{4!}\left(\beta_9 - \frac{1}{9!}\right) - \frac{1}{3!\,10!} - \frac{1}{12!} + \frac{1}{2!\,11!} + \frac{1}{13!}. \end{aligned}$$

3. Derivation of RK pairs with higher orders of dissipation and dispersion

We start constructing a nine-stage family of pairs of explicit RK formulas with algebraic orders seven and five. This means that we have at our disposal the parameters of the lower triangular matrix $A \in \mathbb{R}^{9\times 9}$, and the vectors $\boldsymbol{b} \in \mathbb{R}^9$ and $\boldsymbol{b}^* \in \mathbb{R}^9$, which satisfy the $85 + 17$ order equations (2.5), (2.6). Since the process which leads to the construction of this family is very similar to the one used by the authors in [3] to obtain RK triples, some technical details will be omitted.

First, to simplify this set of equations we assume that A satisfies the well known simplifying assumptions [2]

$$A\boldsymbol{e}_2 = a_{32}\boldsymbol{e}_3, \quad A\boldsymbol{c} = \tfrac{1}{2}(\boldsymbol{c}^2 - c_2^2\boldsymbol{e}_2), \quad A\boldsymbol{c}^2 = \tfrac{1}{3}(\boldsymbol{c}^3 - c_2^3\boldsymbol{e}_2), \tag{3.1}$$

where $\boldsymbol{e} = (1, 1, \ldots, 1)^{\mathrm{T}} \in \mathbb{R}^9$, $\boldsymbol{c} = (c_i) = A\boldsymbol{e}$, $\boldsymbol{e}_j \in \mathbb{R}^9$ is the vector with components $(\boldsymbol{e}_j)_i = \delta_{ij}$ (δ_{ij} is the Kronecker delta) and $\boldsymbol{u}^2 = \boldsymbol{u} \cdot \boldsymbol{u}$, where $\boldsymbol{u} \cdot \boldsymbol{v}$ is the componentwise product of vectors $\boldsymbol{u}$ and $\boldsymbol{v}$, i.e. $(\boldsymbol{u} \cdot \boldsymbol{v})_i = u_i v_i$.

In addition to (3.1) it will be assumed also that the vector $\boldsymbol{b} = (b_i)$ satisfies the equation

$$\boldsymbol{b}^{\mathrm{T}} A = \boldsymbol{b}^{\mathrm{T}} - (\boldsymbol{b} \cdot \boldsymbol{c})^{\mathrm{T}}. \tag{3.2}$$

With the above conditions, it is found after some calculations that the 85 conditions of the seventh order solution are equivalent to $b_2 = b_3 = 0$,

$$\boldsymbol{b}^{\mathrm{T}} \boldsymbol{c}^j = 1/(j+1), \quad j = 0, \ldots, 6 \tag{3.3a}$$

and

$$\begin{aligned} &(\boldsymbol{b} \cdot \boldsymbol{c})^{\mathrm{T}} A \boldsymbol{e}_3 = 0, \quad (\boldsymbol{b} \cdot \boldsymbol{c})^{\mathrm{T}} A \boldsymbol{c}^3 = 1/24, \quad (\boldsymbol{b} \cdot \boldsymbol{c}^2)^{\mathrm{T}} A \boldsymbol{c}^3 = 1/28, \\ &(\boldsymbol{b} \cdot \boldsymbol{c}^2)^{\mathrm{T}} A^3 \boldsymbol{c} = 1/168, \quad (\boldsymbol{b} \cdot \boldsymbol{c})^{\mathrm{T}} A \boldsymbol{c}^4 = 1/35, \\ &(\boldsymbol{b} \cdot \boldsymbol{c})^{\mathrm{T}} A^2 \boldsymbol{c}^3 = 1/140, \quad (\boldsymbol{b} \cdot \boldsymbol{c})^{\mathrm{T}} A^2 \boldsymbol{e}_3 = 0. \end{aligned} \tag{3.3b}$$

Similarly, the simplifying assumptions (3.1) allow to reduce the fifth order conditions (2.5) to $b_2^* = b_3^* = 0$, and

$$(\boldsymbol{b}^*)^{\mathrm{T}} \boldsymbol{c}^j = 1/(j+1), \quad j = 0, \ldots, 4, \tag{3.4}$$

and

$$(\boldsymbol{b}^*)^{\mathrm{T}} A \boldsymbol{c}^3 = 1/20, \qquad (\boldsymbol{b}^*)^{\mathrm{T}} A \boldsymbol{e}_3 = 0. \tag{3.5}$$

After these reductions in the algebraic equations of the order conditions, a closer examination of the simplifying assumptions (3.1), (3.2) and the remaining order conditions (3.3)–(3.5) shows that the components c_i of the vector $\boldsymbol{c}$ satisfy

$$c_1 = 0, \quad c_2 = \tfrac{2}{3} c_3, \quad c_3 = \tfrac{2}{3} c_4, \quad c_9 = 1.$$

In order to construct our RK pairs we have taken c_4, c_6, c_7, c_8 and b_4^* as free parameters, then it can be seen that the remaining coefficients c_5, a_{ij}, b_i and $b_i^* (i \neq 4)$ can be determined successively by using the order equations and the simplifying assumptions, resulting that all equations are finally satisfied. Since this calculation involves lengthy algebraic manipulations its details will be omitted here. It must be remarked that as it is usual in the construction of RK pairs, the value of b_4^* is used to tune appropriately the two formulas of the pair.

In conclusion, for each set of values of the parameters c_4, c_6, c_7, c_8, b_4^* we have a RK pair of formulas of algebraic orders seven and five whose coefficients can be computed explicitly. Moreover the coefficients which appear in the dispersion and dissipation order conditions β_8 and β_9 given by

$$\beta_8 = \beta_8(c_4, c_6, c_7, c_8) = \boldsymbol{b}^{\mathrm{T}} A^7 \boldsymbol{e}, \qquad \beta_9 = \beta_9(c_4, c_6, c_7, c_8) = \boldsymbol{b}^{\mathrm{T}} A^8 \boldsymbol{e},$$

turn out to be rational functions of the free parameters c_4, c_6, c_7, c_8 (its explicit expressions are too lengthy to be reproduced here). Our next task consists in selecting appropriately the values of the free parameters c_4, c_6, c_7, c_8 so that the higher order formula be dispersive and/or dissipative with the highest possible order.

Since all advancing formulas of the above family have algebraic order seven their order of dispersion is $\geqslant 8$ and their order of dissipation $\geqslant 7$. Now we may attempt to increase either the dispersion or dissipation orders or else both at the same time. First, if we want to get dispersive formulas with the highest possible order we should choose β_8 and β_9 so that the coefficients C_9 and C_{11} of $\phi(v)$ given by (2.16) vanish, i.e.

$$\beta_8 = \frac{1}{41580}, \qquad \beta_9 = \frac{1}{498960}, \tag{3.6}$$

with these values we have $C_{13} \neq 0$ and $D_8 \neq 0$, and we would get RK pairs with advancing formulas which are dispersive of order 12 and dissipative of order 7.

As noted above, β_8 and β_9 are nonlinear functions of the free parameters c_4, c_6, c_7, c_8 and the question arises whether the nonlinear equations in the free parameters given by (3.6) possess real solutions in the practical range of values of these parameters. It is found numerically that there exist an infinite set of solutions and then we have proceed by choosing c_4, c_6, c_7, c_8 so that satisfy (3.6) subject to the following constraints: Firstly, to minimize the $|\cdot|_2$–norm of the coefficients of the elementary differentials in the leading term of the local error expansion of the formula (2.2), (2.4). Secondly, that the higher order formula of the pair possess a large stability interval, particularly around the imaginary axis. Thirdly, that the estimate $|y_{n+1} - y^*_{n+1}|$ given by the pair provide a reliable stepsize policy. In this way we have obtained a RK pair denoted by RK[7(5),12,7], corresponding to the values of the parameters

$$c_4 = \frac{571729}{6076042}, \quad c_6 = \frac{2879565}{6539111}, \quad c_7 = \frac{4}{5}, \quad c_8 = \frac{9}{10}, \quad b_4^* = \frac{1}{4}. \tag{3.7}$$

A second possibility is to look for methods with the highest order of dissipation. In this case the methods should be such that the coefficients D_8 and D_{10} of v^8 and v^{10} in the dissipation error function given by (2.18) vanish, i.e. β_8 and β_9 take the values (2.19). There are four parameters c_4, c_6, c_7, c_8 to make β_8 and β_9 satisfy (2.19). We have to proceed as in the above case, arriving at the following values for the parameters:

$$c_4 = \frac{1329760}{10500709}, \quad c_6 = \frac{603240}{1059769}, \quad c_7 = \frac{3}{4}, \quad c_8 = \frac{8}{9}, \quad b_4^* = \frac{1}{4}, \tag{3.8}$$

and the corresponding RK pair will be denoted by RK[7(5),8,11].

Finally, if we want to increase both orders of dissipation and dispersion we may choose β_8 and β_9 so that vanish simultaneously the leading terms in the dispersion and dissipation errors. This is accomplished by

$$\beta_8 = \frac{1}{40320}, \qquad \beta_9 = \frac{1}{362880}, \tag{3.9}$$

and with these values both orders are exactly 10 and 9, respectively. As in the above cases, by using the freedom in the parameters c_4, c_6, c_7, c_8 to minimize the leading coefficients of the local error, the values of these parameters are

$$c_4 = \frac{1}{7}, \quad c_6 = \frac{13}{24}, \quad c_7 = \frac{7}{9}, \quad c_8 = \frac{91}{100}, \quad b_4^* = \frac{1}{4}, \tag{3.10}$$

Table 1

Method	Leading term dispersion error	Leading term dissipation error
RK[7(5),12,7]	$-1.0278 \times 10^{-8}\ v^{13}$	$7.5156 \times 10^{-7}\ v^{8}$
RK[7(5),10,9]	$2.5052 \times 10^{-7}\ v^{11}$	$-2.7557 \times 10^{-7}\ v^{10}$
RK[7(5),8,11]	$2.7557 \times 10^{-7}\ v^{9}$	$6.8893 \times 10^{-8}\ v^{12}$
DOPRI8(7)	$3.6039 \times 10^{-9}\ v^{9}$	$-2.9649 \times 10^{-8}\ v^{10}$
RKF8(7)	$4.0660 \times 10^{-7}\ v^{9}$	$3.6729 \times 10^{-7}\ v^{10}$

and the method is denoted by RK[7(5),10,9]. The Butcher's array of the coefficients of this pair is given in the Appendix.

To end this section we present some additional features of our new methods. First of all we show in Table 1 the leading terms of the dispersion and dissipation error functions of the new methods and their corresponding for the higher order solutions of Felhberg [4] (RKF 8(7)) and Prince and Dormand [7] (DOPRI 8(7)) pairs given in powers of $v = h\omega$.

As can be seen the three new methods compare favourably with Felberg's method. However, the pair of Prince and Dormand has smaller error constants, particularly for the dispersion error, this means the new methods will be comparable only for small values of v.

On the other hand, we have compared the dispersion ($\phi(v)$) and dissipation ($\alpha(v)$) error functions of our three methods on a finite range of values of v. To illustrate the behaviour of these functions we show in Figs. 1(a) and (b) the graphs of the logarithm of these functions in terms of v for $v \leqslant 4$ (the approximate limit of stability region on the imaginary axis). As can be seen in these figures, if both dispersion and dissipation are considered for the selection of the most convenient formula, the RK [7(5), 10, 9] is probably the best choice.

Finally, as far as the stability of the new methods is concerned, let us note that the choice of the available parameters of the new pairs was carried out taking into account the stability behaviour of the higher order formula, particularly around the imaginary axis. In Fig. 2 we show the stability regions of the new methods. It follows from these figures that the stability region of the RK [7(5), 10, 9] method contains the larger stability interval on the imaginary axis. Moreover, as can be seen in [7] this interval is also larger than the corresponding to RKF8(7) and DOPRI8(7) methods.

4. Numerical results

To test the efficiency of the new methods in the numerical solution of problems with oscillating solutions we have compared the behaviour of variable stepsize codes based on these formulae with similar codes based on the well known higher order pairs of Fehlberg RKF8(7) [4] and of Prince and Dormand of orders 8 and 7 [7]. Although Fehlberg and Prince and Dormand pairs have higher algebraic orders than our pairs we have chosen them as a reference test because they are widely employed in high precision calculations and the conclusions derived from these comparisons can be more useful for people interested in practical computation.

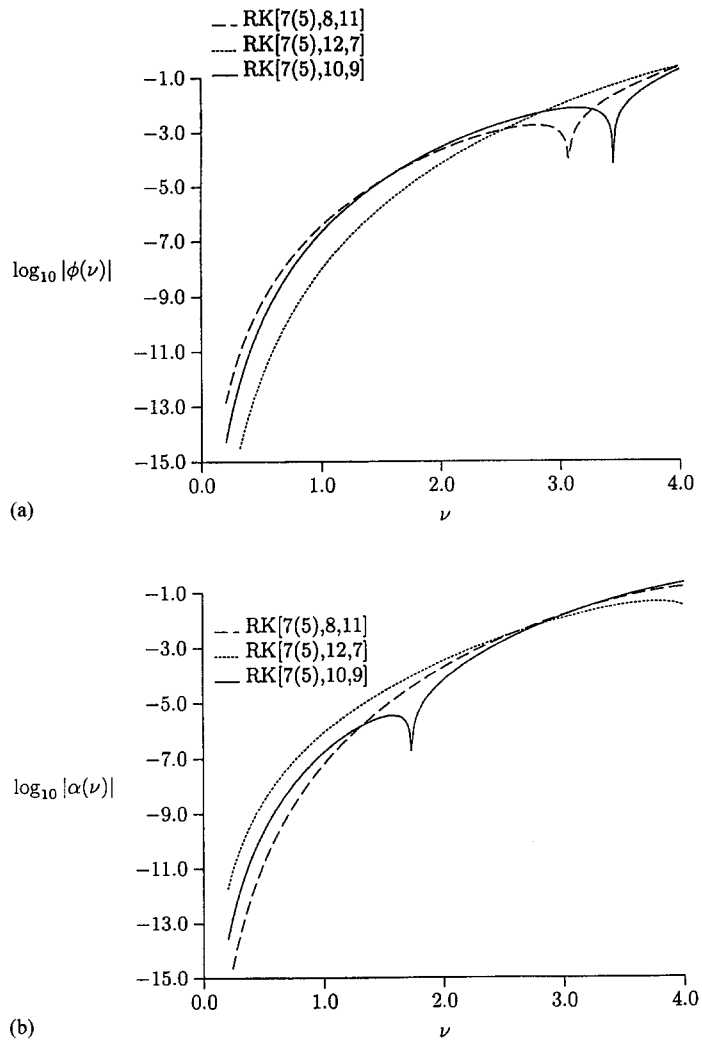


Fig. 1. (a) Dispersion error.

When undertaking a comparison between methods it is obviously very important the criterion to be used in this comparison. Thus, in some numerical tests carried out in [10], a comparison between several methods has been based exclusively on their ability to locate a certain zero of a given component of the numerical solution or else in finding the number of zeros in a given interval. In our opinion, such a test reveals only a particular feature of the numerical solution provided by the method as it is the capability to stay in phase. Therefore we have decided to employ the usual test based in the comparison of the numerical and theoretical solutions on the grid points (which are defined by the numerical method for each given tolerance) whenever an analytical expression for its solution is known or a comparison on previously selected points otherwise.

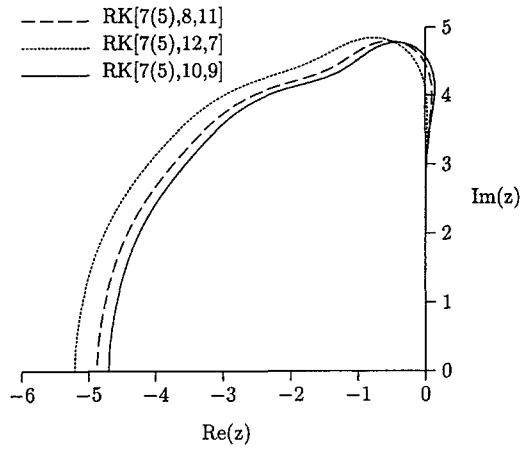


Fig. 2. Stability regions.

As test problems we have considered several model and nonmodel problems with linear and nonlinear oscillations and different dimensions, here we present only some numerical results of four problems:

Problem 4.1. The linear homogeneous model problem is given by

$$y' = \begin{pmatrix} 0 & 10 \\ -10 & 0 \end{pmatrix} y, \quad y(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

in the interval $[0, 1000]$, whose exact solution is $y(t) = (\cos(10t), \sin(10t))^{\mathrm{T}}$.

Problem 4.2. The linear nonhomogeneous problem with a periodic forcing term

$$y' = \begin{pmatrix} 0 & 1 \\ -100 & 0 \end{pmatrix} y + \begin{pmatrix} 0 \\ 99 \sin t \end{pmatrix}, \quad y(0) = \begin{pmatrix} 1 \\ 11 \end{pmatrix},$$

in the interval $[0, 1000]$. The exact solution is $y(t) = (\varphi(t), \varphi'(t))^{\mathrm{T}}$ with $\varphi(t) = \cos(10t) + \sin(10t) + \sin t$.

Problem 4.3. The linear homogeneous system with dimension 50 which arises in the spatial discretization of a first order hyperbolic equation (see [10] for a complete description of the problem), given by

$$y' = \frac{1}{2\Delta x} \begin{pmatrix} 0 & 1 & & & \\ 1 & 0 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 0 & -1 \\ & & -1 & 4 & -3 \end{pmatrix} y, \qquad y \in \mathbb{R}^{50},$$

where $\Delta x = 1/50$ and $y(0) = (y_j)$ with $y_j = \sin(\pi j \Delta x)^2$. This problem is considered in the interval $[0, 33.509996948]$ and its numerical solution is tested only at the end point of the interval.

Problem 4.4. We consider a spatial discretization of the first order hyperbolic system

$$\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}-v\frac{\partial u}{\partial x}-\omega u=0, \qquad \frac{\partial u}{\partial t}+u\frac{\partial v}{\partial x}-v\frac{\partial u}{\partial x}+\omega v=0,$$

with the initial and boundary conditions

$$v(0,t)=u(0,t)=0, \quad t>0, \qquad v(x,0)=0, \; u(x,0)=a(x), \quad 0<x<1.$$

Here the initial and boundary conditions have been chosen so that the problem has the solution

$$v(x,t)=a(x)\,\sin(\omega t), \qquad u(x,t)=a(x)\cos(\omega t),$$

with $a(x)=x(x-1)$.

Let $x_i=i\Delta x$, $i=1,\ldots,N$, with $N\Delta x=1$ be an spatial equidistant grid on $[0,1]$. We approximate the spatial derivatives by using second order symmetric differences at internal grid points and one-sided differences at the boundary point $x=1$. Putting $v_j(t)=v(x_j,t)$ and $u_j(t)=u(x_j,t)$ we arrive to the following system of differential equations:

$$\begin{aligned}
v_1' &= -\frac{v_1u_2}{2\Delta x}+\frac{u_1v_2}{2\Delta x}+\omega u_1,\\
v_j' &= v_j\frac{u_{j-1}-u_{j+1}}{2\Delta x}-u_j\frac{v_{j-1}-v_{j+1}}{2\Delta x}+\omega u_j, \quad (j=2,3\ldots,N-1),\\
v_N' &= v_N\frac{u_{N-2}-4u_{N-1}+3u_N}{2\Delta x}-u_N\frac{v_{N-2}-4v_{N-1}+3v_N}{2\Delta x}+\omega u_N,\\
u_1' &= -\frac{v_1u_2}{2\Delta x}+\frac{u_1v_2}{2\Delta x}-\omega v_1,\\
u_j' &= v_j\frac{u_{j-1}-u_{j+1}}{2\Delta x}-u_j\frac{v_{j-1}-v_{j+1}}{2\Delta x}-\omega v_j, \quad (j=2,3\ldots,N-1)\\
u_N' &= v_N\frac{u_{N-2}-4u_{N-1}+3u_N}{2\Delta x}-u_N\frac{v_{N-2}-4v_{N-1}+3v_N}{2\Delta x}-\omega v_N.
\end{aligned}$$

with the initial conditions

$$v_j(0)=0, \qquad u_j(0)=a(x_j), \quad j=1,\ldots,N.$$

Due to the special solution considered here the analytical solution of the discretized problem is also known in advance and this fact makes easier to check numerically the behaviour of the methods.

To make the numerical comparisons independent of the implementations we have started with a well tested code similar to DOPRI8 [5], and we have modified it by substituting the pair of Prince and Dormand by the new pairs constructed in the previous section and changing the stepsize control according to the algebraic orders of the new formulae. All computations have been carried out in double precision (15 digits) in an ALPHA AXP system of the University of Zaragoza.

Our first aim was to investigate numerically, in the context of our family of RK7(5) pairs, whether the code with the optimum pair RK[7(5), 12, 7] with highest order of dispersion performed better than the code with highest order of dissipation RK[7(5), 8, 11] or else the code with the more equilibrated dispersion–dissipation pair RK[7(5), 10, 9]. Then, we have computed for a given

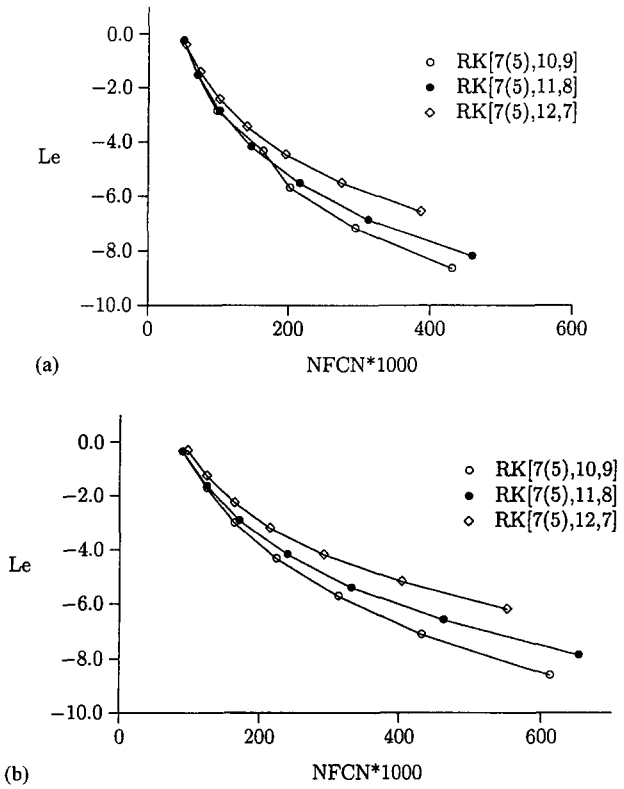
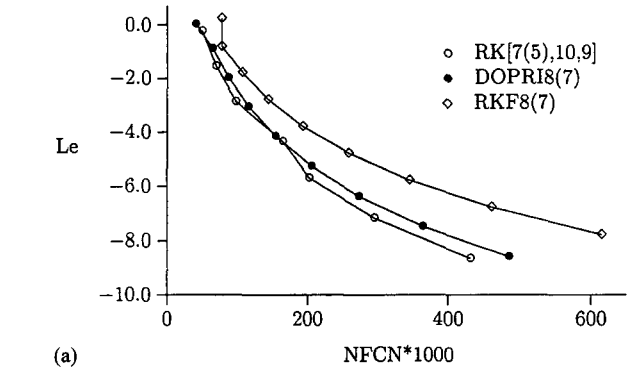


Fig. 3. (a). Problem 4.1 and (b) Problem 4.2.

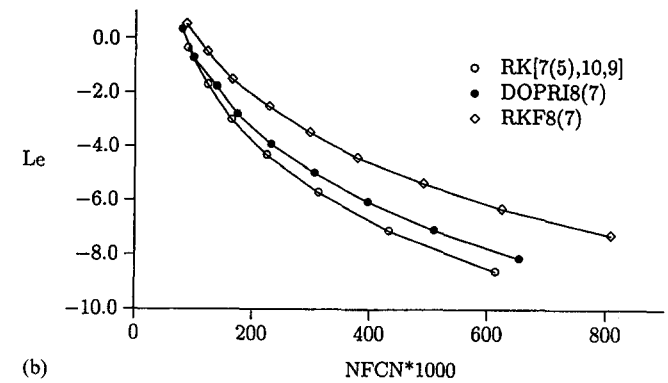
tolerance (usually in the range 10^{-j}, $j = 3,\ldots,10$) the logarithm of the max. norm of the global error (Le) over the whole integration interval and the computational cost measured by the number of function evaluations (NFCN) for several problems test. In this way we may plot, for each method, a polygonal joining the points (NFCN, Le) obtained for all tolerances and the computational cost required to get a given max. global error is clearly displayed.

In Figs. 3(a) and (b) we have plotted the efficiency curves for the three methods and the Problems 4.1 and 4.2, respectively. As can be seen in these graphs the code which uses the pair RK[7(5), 10, 9] is clearly superior to the other pairs. This fact is also supported by other numerical experiments not presented here. In view of these results we may conclude that the pair RK[7(5),10, 9] is the most convenient method for problems with oscillating solutions, particularly at stringent tolerances.

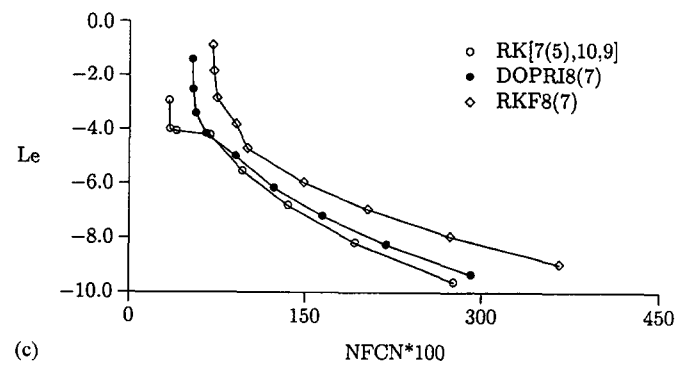
After this selection within our family of methods, we have compared the numerically optimal new pair RK[7(5), 10, 9] with the well-known RKF8(7) and DOPRI8(7). The tests employed have been the same as above and in Figs 4(a)–(c) we show the efficiency curves of the three methods for the Problems 4.1–4.3, respectively. A first noticeable fact that follows from the above graphs is that the new method performs better for all tolerances than the other classical pairs although it has a lower algebraic order. In addition this difference becomes, in many cases, more significant at stringent tolerances.



(a)



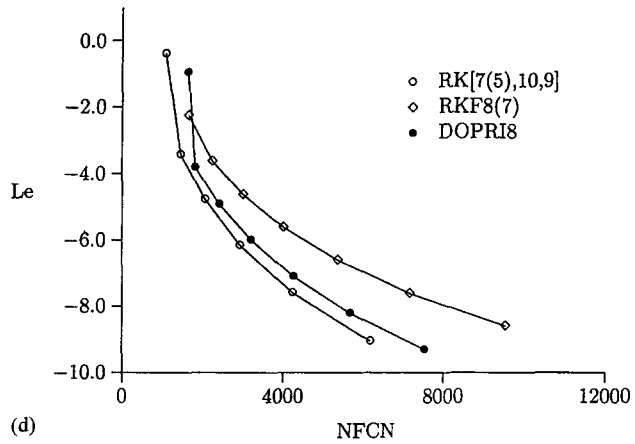
(b)



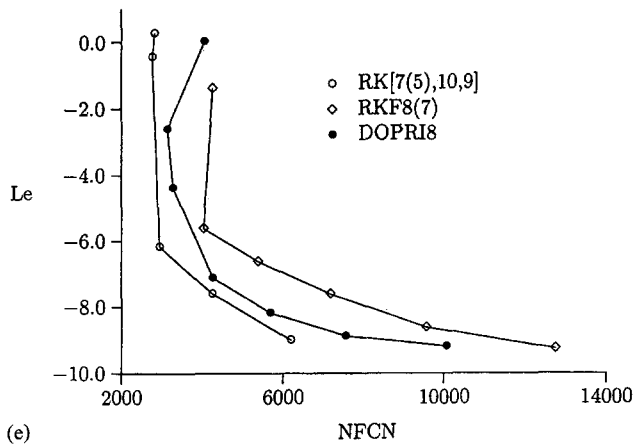
(c)

Fig. 4. (a) Problem 4.1, (b) Problem 4.2 (c) Problem 4.3.

Finally, in Figs. 4(d) and (e) we present the numerical results obtained with RK[7(5), 10,9], DOPRI8(7) and RKF8(7) for the Problem 4.4. These results have been computed at $t_{\text{end}} = 20$ with $\omega = 10$ and values of the discretization parameter $N = 10, 20$. The information displayed in this figures reveals again a satisfactory performance of the pair RK[7(5),10,9] which compares favourably with DOPRI8(7) and RKF8(7) pairs.



(d)



(e)

Fig. 4. (d) Problem 4.4, $N = 10$ and (e) Problem 4.5, $N = 20$.

5. Conclusions

We have constructed a family of RK pairs with nine stages and algebraic orders seven and five depending on five parameters. We have selected within this family three optimal pairs attending the criteria of accuracy, stability, reliability of stepsize estimator and the orders of dispersion and/or dissipation.

Taking into account the results of an extensive set of numerical experiments, we have found that the new pair denoted by RK[7(5), 10, 9], which is dispersive of order 10 and dissipative of order 9, is the most efficient among the three selected pairs.

Finally, a comparison of the new pair with the well–known pairs RKF8(7) and DOPRI8(7) has shown its efficiency for the numerical solution of first order differential systems with oscillating solutions. Thus, we may conclude that the new method is very convenient for the numerical solution of this kind of problems.

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References

[1] L. Brusa and L. Nigro, A one step method for direct integration of structural dynamic equations, *Internat. J. Numer. Methods Eng.* **15** (1980) 685–699.
[2] J.C. Butcher, *The Numerical Analysis of Ordinary Differential Equations* (Runge–Kutta and General Linear Methods) (Wiley, New York, 1987).
[3] M. Calvo, J.I. Montijano and L. Rández, A polyvalent Runge–Kutta triple, *Appl. Numer. Math.* **15** (1994) 13–26.
[4] E. Fehlberg, Classical fifth, sixth, seventh and eighth order Runge–Kutta formulas with stepsize control, *NASA Tech. report* R-287 1968.
[5] E. Hairer, S.P. Norsett and G. Wanner, *Solving Ordinary Differential Equations I. Non-stiff Problems* (Springer, Berlin, 1987).
[6] F.Q. Hu, M.Y. Hussaini and J.L. Manthey, Low-dissipation and low-dispersion Runge–Kutta schemes for computational acoustics, *J. Comput. Phy.* **124** (1996) 177–191.
[7] P.J. Prince and J.R. Dormand, High order embedded Runge–Kutta formulae, *J. Comput. Appl. Math.* **7** (1981) 67–75.
[8] P.W. Sharp, J.M. Fine and K. Burrage, Two-stage and three-stage diagonally implicit Runge–Kutta–Nyström methods of orders three and four, *IMA J. Numer. Anal.* **10** (1990) 489–504.
[9] A.B. Sideris and T.E. Simos, A low-order embedded Runge–Kutta method for periodic initial-value problems, *J. Comput. Appl. Math.* **44** (1992) 235–244.
[10] P.J. Van der Houwen and B.P. Sommeijer, Explicit Runge–Kutta (Nyström) methods with reduced phase errors for computing oscillating solutions, *SIAM J. Numer. Anal.* **24** (1987) 595–617.
[11] P.J. Van der Houwen and B.P. Sommeijer, Phase-lag analysis of implicit Runge–Kutta methods, *SIAM J. Numer. Anal.* **26** (1989) 214–229.
[12] P.J. Van der Houwen and B.P. Sommeijer, Diagonally implicit Runge–Kutta–Nyström methods for oscillatory problems, *SIAM J. Numer. Anal.* **26** (1989) 414–429.
[13] P.J. Van der Houwen, B.P. Sommeijer, K. Strehmel and R. Weiner, On the numerical integration of second-order initial value problems with a periodic forcing function, Tech. Report NM-R8604, Center for Mathematics and Computer Science, Amsterdam, The Netherlands, 1986.

Appendix. RK[7(5), 10,9]

0									
$\frac{4}{63}$	$\frac{4}{63}$								
$\frac{2}{21}$	$\frac{1}{42}$	$\frac{1}{14}$							
$\frac{1}{7}$	$\frac{1}{28}$	0	$\frac{3}{28}$						
$\frac{1}{7}$	$\frac{1}{28}$	0	$\frac{3}{28}$						
$\frac{7}{17}$	$\frac{12551}{19652}$	0	$\frac{-48363}{19652}$	$\frac{10976}{4913}$					
$\frac{13}{24}$	$\frac{-36616931}{27869184}$	0	$\frac{2370277}{442368}$	$\frac{-255519173}{63700992}$	$\frac{226798819}{445906944}$				
$\frac{7}{9}$	$\frac{-10401401}{7164612}$	0	$\frac{47383}{8748}$	$\frac{-4914455}{1318761}$	$\frac{-1498465}{7302393}$	$\frac{2785280}{3739203}$			
$\frac{91}{100}$	$\frac{181002080831}{17500000000}$	0	$\frac{-14827049601}{400000000}$	$\frac{23296401527134463}{857600000000000}$	$\frac{2937811552328081}{949760000000000}$	$\frac{-243874470411}{69355468750}$	$\frac{2857867601589}{3200000000000}$		
1	$\frac{-228380759}{19257212}$	0	$\frac{4828803}{113948}$	$\frac{-331062132205}{10932626912}$	$\frac{-12727101935}{3720174304}$	$\frac{226272053145 60}{4940625496417}$	$\frac{-268403949}{461033608}$	$\frac{3600000000000}{19176750553961}$	
order 7	$\frac{95}{2366}$	0	0	$\frac{3822231133}{16579123200}$	$\frac{555164087}{2298419200}$	$\frac{1279328256}{9538891505}$	$\frac{5963949}{25894400}$	$\frac{50000000000}{599799373173}$	$\frac{28487}{712800}$
order 5	$\frac{1689248233}{50104356120}$	0	0	$\frac{1}{4}$	$\frac{28320758959727}{152103780259200}$	$\frac{66180849792}{341834007515}$	$\frac{31163653341}{152322513280}$	$\frac{362415118750 00}{394222326561063}$	$\frac{28487}{712800}$